```
$%^STN;HighlightOn=  ***;HighlightOff=***  ;

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 NEWS  1          Web Page for STN Seminar Schedule - N. America
 NEWS  2  MAR 31  IFICDB, IFIPAT, and IFIUDB enhanced with new custom
                  IPC display formats
 NEWS  3  MAR 31  CAS REGISTRY enhanced with additional experimental
                  spectra
 NEWS  4  MAR 31  CA/CAplus and CASREACT patent number format for U.S.
                  applications updated
 NEWS  5  MAR 31  LPCI now available as a replacement to LDPCI
 NEWS  6  MAR 31  EMBASE, EMBAL, and LEMBASE reloaded with enhancements
 NEWS  7  APR 04  STN AnaVist, Version 1, to be discontinued
 NEWS  8  APR 15  WPIDS, WPINDEX, and WPIX enhanced with new
                  predefined hit display formats
 NEWS  9  APR 28  EMBASE Controlled Term thesaurus enhanced
 NEWS 10  APR 28  IMSRESEARCH reloaded with enhancements
 NEWS 11  MAY 30  INPAFAMDB now available on STN for patent family
                  searching
 NEWS 12  MAY 30  DGENE, PCTGEN, and USGENE enhanced with new homology
                  sequence search option
 NEWS 13  JUN 06  EPFULL enhanced with 260,000 English abstracts
 NEWS 14  JUN 06  KOREAPAT updated with 41,000 documents
 NEWS 15  JUN 13  USPATFULL and USPAT2 updated with 11-character
                  patent numbers for U.S. applications
 NEWS 16  JUN 19  CAS REGISTRY includes selected substances from
                  web-based collections
 NEWS 17  JUN 25  CA/CAplus and USPAT databases updated with IPC
                  reclassification data
 NEWS 18  JUN 30  AEROSPACE enhanced with more than 1 million U.S.
                  patent records
 NEWS 19  JUN 30  EMBASE, EMBAL, and LEMBASE updated with additional
                  options to display authors and affiliated
                  organizations
 NEWS 20  JUN 30  STN on the Web enhanced with new STN AnaVist
                  Assistant and BLAST plug-in
 NEWS 21  JUN 30  STN AnaVist enhanced with database content from EPFULL
 NEWS 22  JUL 28  CA/CAplus patent coverage enhanced
 NEWS 23  JUL 28  EPFULL enhanced with additional legal status
                  information from the epoline Register
 NEWS 24  JUL 28  IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
 NEWS 25  JUL 28  STN Viewer performance improved
```

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 NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
              AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8

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FILE 'HOME' ENTERED AT 06:48:25 ON 29 JUL 2008

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

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STRUCTURE FILE UPDATES:   28 JUL 2008  HIGHEST RN 1036756-19-0
DICTIONARY FILE UPDATES:  28 JUL 2008  HIGHEST RN 1036756-19-0

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=>
Uploading C:\Program Files\STNEXP\Queries\10535043.str

L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
```

```
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l1
SAMPLE SEARCH INITIATED 06:49:49 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -        7 TO ITERATE

100.0% PROCESSED        7 ITERATIONS                                 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            7 TO      298
PROJECTED ANSWERS:               2 TO      124

L2            2 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 06:50:15 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      134 TO ITERATE

100.0% PROCESSED      134 ITERATIONS                               10 ANSWERS
SEARCH TIME: 00.00.01

L3           10 SEA SSS FUL L1

=> d scan

L3   10 ANSWERS   REGISTRY  COPYRIGHT 2008 ACS on STN
IN   2-Propenoic acid, 3-[3-[[[2-(acetyloxy)-4-(3-butoxy-3-oxo-1-propen-1-
     yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester
MF   C33 H39 N O7


/ Structure 1 in file .gra /


**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3   10 ANSWERS   REGISTRY  COPYRIGHT 2008 ACS on STN
IN   2-Propenoic acid, 3-[3-[[[4-(3-butoxy-3-oxo-1-propen-1-yl)-2-(2-ethoxy-2-
     oxoethoxy)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester
MF   C35 H43 N O8



/ Structure 2 in file .gra /
```

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file cap
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 179.28 | 179.49

FILE 'CAPLUS' ENTERED AT 06:51:03 ON 29 JUL 2008
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FILE COVERS 1907 - 29 Jul 2008 VOL 149 ISS 5
FILE LAST UPDATED: 28 Jul 2008 (20080728/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

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=> s l3
L4 1 L3

=> d ibib abs hitstr

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:382121 CAPLUS <<LOGINID::20080729>>
DOCUMENT NUMBER: 147:22696
TITLE: 3D-QSAR studies with the aid of molecular docking for a series of non-steroidal FXR agonists
AUTHOR(S): Zhang, Tao; Zhou, Jun-Hong; Shi, Liang-Wei; Zhu, Rui-Xin; Chen, Min-Bo
CORPORATE SOURCE: Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China
SOURCE: Bioorganic & Medicinal Chemistry Letters (2007), 17(8), 2156-2160
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The farnesoid x receptor (FXR) has become a potential drug target for treating cholesterol-related and bile acid-related diseases recently. In this paper, 3-dimensional quant. structure-activity (structure-affinity and structure-efficacy) relationships are investigated for a series of nonsteroidal agonists (fexaramine series) by using the comparative mol. field anal. (Co-MFA), where mol. docking method (FlexX) is employed to construct mol. superimposition maps. A proposal to design some new agonists is discussed lastly.
IT ***938197-65-0*** ***938197-67-2*** ***938197-86-5***
938197-97-8 ***938197-98-9*** ***938197-99-0***
938198-00-6 ***938198-01-7*** ***938198-02-8***
938198-03-9
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(mol. docking and 3D-QSAR for a series of non-steroidal FXR agonists)
RN 938197-65-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(3-butoxy-3-oxo-1-propen-1-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 3 in file .gra /

RN 938197-67-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(3-butoxy-3-oxo-1-propen-1-yl)phenyl]methyl](2-naphthalenylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 4 in file .gra /

RN 938197-86-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[benzoyl[[4-(3-butoxy-3-oxo-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 5 in file .gra /

RN 938197-97-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(3-butoxy-3-oxo-1-propen-1-yl)-2-hydroxyphenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 6 in file .gra /

RN 938197-98-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(3-butoxy-3-oxo-1-propen-1-yl)-2-methoxyphenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 7 in file .gra /

RN 938197-99-0 CAPLUS

CN 2-Propenoic acid, 3-[3-[[[4-(3-butoxy-3-oxo-1-propen-1-yl)-2-(phenylmethoxy)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 8 in file .gra /

RN 938198-00-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[2-(acetyloxy)-4-(3-butoxy-3-oxo-1-propen-1-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 9 in file .gra /

RN 938198-01-7 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[2-(benzoyloxy)-4-(3-butoxy-3-oxo-1-propen-1-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 10 in file .gra /

RN 938198-02-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(3-butoxy-3-oxo-1-propen-1-yl)-2-[(methylsulfonyl)oxy]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 11 in file .gra /

RN 938198-03-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(3-butoxy-3-oxo-1-propen-1-yl)-2-(2-ethoxy-2-oxoethoxy)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 12 in file .gra /

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file logoff
'LOGOFF' IS NOT A VALID FILE NAME
SESSION CONTINUES IN FILE 'CAPLUS'
Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

=> file stng

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	7.37	186.86

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL

```
                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                    -0.80      -0.80

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COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                     ENTRY    SESSION
FULL ESTIMATED COST                                   0.12     186.98

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)      SINCE FILE      TOTAL
                                                     ENTRY    SESSION
CA SUBSCRIBER PRICE                                   0.00      -0.80

FILE 'REGISTRY' ENTERED AT 06:54:55 ON 29 JUL 2008
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STRUCTURE FILE UPDATES:   28 JUL 2008  HIGHEST RN 1036756-19-0
DICTIONARY FILE UPDATES:  28 JUL 2008  HIGHEST RN 1036756-19-0

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http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\STNEXP\Queries\10535043 take 2.str

L5      STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5              STR

/ Structure 13 in file .gra /


Structure attributes must be viewed using STN Express query preparation.
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```
=> s l5 sss sam
SAMPLE SEARCH INITIATED 06:55:22 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      123 TO ITERATE

100.0% PROCESSED      123 ITERATIONS                                3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         1795 TO     3125
PROJECTED ANSWERS:               3 TO      162

L6            3 SEA SSS SAM L5

=> s l5 sss ful
FULL SEARCH INITIATED 06:55:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     2524 TO ITERATE

100.0% PROCESSED     2524 ITERATIONS                               90 ANSWERS
SEARCH TIME: 00.00.01

L7           90 SEA SSS FUL L5

=> file cap
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     178.36     365.34

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                       0.00      -0.80

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FILE COVERS 1907 - 29 Jul 2008  VOL 149 ISS 5
FILE LAST UPDATED: 28 Jul 2008  (20080728/ED)

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=> s l7
L8   13 L7

=> d 1-13 ibib abs hitstr

L8   ANSWER 1 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:382121 CAPLUS <<LOGINID::20080729>>
DOCUMENT NUMBER: 147:22696
TITLE: 3D-QSAR studies with the aid of molecular docking for a series of non-steroidal FXR agonists
AUTHOR(S):   Zhang, Tao; Zhou, Jun-Hong; Shi, Liang-Wei; Zhu, Rui-Xin; Chen, Min-Bo
CORPORATE SOURCE: Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China
SOURCE: Bioorganic & Medicinal Chemistry Letters (2007), 17(8), 2156-2160
                         CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB   The farnesoid x receptor (FXR) has become a potential drug target for treating cholesterol-related and bile acid-related diseases recently. In this paper, 3-dimensional quant. structure-activity (structure-affinity and structure-efficacy) relationships are investigated for a series of nonsteroidal agonists (fexaramine series) by using the comparative mol. field anal. (Co-MFA), where mol. docking method (FlexX) is employed to construct mol. superimposition maps. A proposal to design some new agonists is discussed lastly.
IT   ***574013-66-4*** ***574013-67-5*** ***574013-68-6***
     592525-03-6 ***592525-04-7*** ***592525-05-8***
     592525-07-0 ***592525-08-1*** ***592525-09-2***
     592525-10-5 ***592525-21-8*** ***592525-25-2***
     592525-26-3 ***592525-27-4*** ***592525-28-5***
     592525-29-6 ***592525-32-1*** ***592525-35-4***
     592525-38-7 ***592525-41-2*** ***592525-44-5***
     592525-47-8 ***592525-50-3*** ***592525-55-8***
     592525-58-1 ***592525-61-6*** ***592525-64-9***
     592525-67-2 ***592525-72-9*** ***592525-78-5***
     592525-81-0 ***592525-84-3*** ***592525-87-6***
     592525-90-1 ***592525-93-4*** ***592525-98-9***
     592526-01-7 ***592526-04-0*** ***592526-07-3***
     592526-12-0 ***938197-64-9*** ***938197-65-0***
     938197-67-2 ***938197-74-1*** ***938197-75-2***
     938197-76-3 ***938197-77-4*** ***938197-78-5***
     938197-79-6 ***938197-80-9*** ***938197-81-0***
     938197-82-1 ***938197-86-5*** ***938197-92-3***
     938197-93-4 ***938197-95-6*** ***938197-96-7***
     RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (mol. docking and 3D-QSAR for a series of non-steroidal FXR agonists)
RN   574013-66-4 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(dimethylamino)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 14 in file .gra /

RN 574013-67-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(1,3-benzodioxol-5-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 15 in file .gra /

RN 574013-68-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(2-phenylethenyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 16 in file .gra /

RN 592525-03-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(2-carboxyethenyl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, 1-methyl ester (CA INDEX NAME)

/ Structure 17 in file .gra /

RN 592525-04-7 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 18 in file .gra /

RN 592525-05-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-ethoxy-3-oxo-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 19 in file .gra /

RN 592525-07-0 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, phenylmethyl ester (CA INDEX NAME)

/ Structure 20 in file .gra /

RN 592525-08-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[3-(dimethylamino)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 21 in file .gra /

RN 592525-09-2 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-methoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 22 in file .gra /

RN 592525-10-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-ethoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 23 in file .gra /

RN 592525-21-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 24 in file .gra /

RN 592525-25-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(5-methyl-2-thienyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 25 in file .gra /

RN 592525-26-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(5-acetyl-2-thienyl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 26 in file .gra /

RN 592525-27-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methoxyphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 27 in file .gra /

RN 592525-28-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-[4-(1,1-dimethylethyl)phenyl]ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 28 in file .gra /

RN 592525-29-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methylphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 29 in file .gra /

RN 592525-32-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2,6-dichlorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 30 in file .gra /

RN 592525-35-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-[2-(3-chlorophenyl)ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 31 in file .gra /

RN 592525-38-7 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-[2-[3,5-bis(trifluoromethyl)phenyl]ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 32 in file .gra /

RN 592525-41-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-[3-(trifluoromethyl)phenyl]ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 33 in file .gra /

RN 592525-44-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2,6-difluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 34 in file .gra /

RN 592525-47-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 35 in file .gra /

RN 592525-50-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2,4,6-trimethylphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 36 in file .gra /

RN 592525-55-8 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(3-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 37 in file .gra /

RN 592525-58-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 38 in file .gra /

RN 592525-61-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2-pyridinyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 39 in file .gra /

RN 592525-64-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methyl-5-thiazolyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 40 in file .gra /

RN 592525-67-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3',4'-difluoro[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 41 in file .gra /

RN 592525-72-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(2'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 42 in file .gra /

RN 592525-78-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-ethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 43 in file .gra /

RN 592525-81-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 44 in file .gra /

RN 592525-84-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(3'-chloro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 45 in file .gra /

RN 592525-87-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 46 in file .gra /

RN 592525-90-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 47 in file .gra /

RN 592525-93-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(5'-chloro-2'-methoxy[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 48 in file .gra /

RN 592525-98-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(3'-chloro-4'-fluoro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 49 in file .gra /

RN 592526-01-7 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 50 in file .gra /

RN 592526-04-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 51 in file .gra /

RN 592526-07-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(2',6'-dimethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 52 in file .gra /

RN 592526-12-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(1,1-dimethylethyl)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 53 in file .gra /

RN 938197-64-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(5-cyclohexyl-2-thienyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 54 in file .gra /

RN 938197-65-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(3-butoxy-3-oxo-1-propen-1-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 55 in file .gra /

RN 938197-67-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(3-butoxy-3-oxo-1-propen-1-yl)phenyl]methyl](2-naphthalenylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 56 in file .gra /

RN 938197-74-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-[4-(methylthio)phenyl]ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 57 in file .gra /

RN 938197-75-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(3-methoxyphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 58 in file .gra /

RN 938197-76-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-[2-(3-acetylphenyl)ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 59 in file .gra /

RN 938197-77-4 CAPLUS

CN 2-Propenoic acid, 3-[3-[[[4-(3-butoxy-3-oxo-1-propen-1-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, ethyl ester (CA INDEX NAME)

/ Structure 60 in file .gra /

RN 938197-78-5 CAPLUS
CN 2-Propenoic acid, 3-[4-[[[3-(3-butoxy-3-oxo-1-propen-1-yl)phenyl](cyclohexylcarbonyl)amino]methyl]phenyl]-, butyl ester (CA INDEX NAME)

/ Structure 61 in file .gra /

RN 938197-79-6 CAPLUS
CN 2-Propenoic acid, 3-[4-[[[3-(3-amino-3-oxo-1-propen-1-yl)phenyl](cyclohexylcarbonyl)amino]methyl]phenyl]-, butyl ester (CA INDEX NAME)

/ Structure 62 in file .gra /

RN 938197-80-9 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, butyl ester (CA INDEX NAME)

/ Structure 63 in file .gra /

RN 938197-81-0 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-ethoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, butyl ester (CA INDEX NAME)

/ Structure 64 in file .gra /

RN 938197-82-1 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-phenoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, butyl ester (CA INDEX NAME)

/ Structure 65 in file .gra /

RN 938197-86-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[benzoyl[[4-(3-butoxy-3-oxo-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 66 in file .gra /

RN 938197-92-3 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, propyl ester (CA INDEX NAME)

/ Structure 67 in file .gra /

RN 938197-93-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-[3-(butylamino)-3-oxo-1-propen-1-yl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 68 in file .gra /

RN 938197-95-6 CAPLUS
CN Benzenepropanoic acid, 4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]-, butyl ester (CA INDEX NAME)

/ Structure 69 in file .gra /

RN 938197-96-7 CAPLUS
CN Benzenepropanoic acid, 4-[[[3-(3-butoxy-3-oxo-1-propen-1-yl)phenyl](cyclohexylcarbonyl)amino]methyl]-, butyl ester (CA INDEX NAME)

/ Structure 70 in file .gra /

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:331294 CAPLUS <<LOGINID::20080729>>
DOCUMENT NUMBER: 148:419
TITLE: Comparative studies of prediction of herb-based FXR ligands by 11 binding free energies scoring functions
AUTHOR(S): Wei, Zhu; Qin, Huang; Li, Xudong; Chen, Keji; Xu, Xiaojie
CORPORATE SOURCE: Guangdong Hospital of Traditional Chinese Medicine, Guangzhou, 510106, Peop. Rep. China
SOURCE: Jisuanji Yu Yingyong Huaxue (2007), 24(1), 94-96
CODEN: JYYHE6; ISSN: 1001-4160
PUBLISHER: Jisuanji Yu Yingyong Huaxue Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB Based on the optimized complex structure of FXR bound with specific ligand-fexaramine (PDB code 1OSH), computer-aided structure-based virtual screening against Peking University Drug Design System (PKUDDS) was conducted to det. the occurrence of herb-based FXR ligands. 11 Scoring functions (igscore1, Ligscore2, D-Score, -PLP1, -PLP2, Jain, -PMF, Ludi1, Ludi2, Ludi3 and consensus) have been compared to evaluate their prediction ability after conformational sampling by program Ligandfit. The results suggest that -PLP1 and -PLP2 have better prediction ability than others.
IT ***574013-66-4*** , Fexaramine
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(comparative studies of prediction of herb-based FXR ligands by 11 binding free energies scoring functions)
RN 574013-66-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(dimethylamino)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 71 in file .gra /

L8 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:157205 CAPLUS <<LOGINID::20080729>>
DOCUMENT NUMBER: 146:434160
TITLE: 3D QSAR comparative molecular field analysis on nonsteroidal farnesoid X receptor activators
AUTHOR(S): Honorio, Kathia M.; Garratt, Richard C.; Polikarpov, Igor; Andricopulo, Adriano D.
CORPORATE SOURCE: Laboratorio de Quimica Medicinal e Computacional, Centro de Biotecnologia Molecular Estrutural, Instituto de Fisica de Sao Carlos, Universidade de Sao Paulo, Sao Carlos, SP, 13560-970, Brazil
SOURCE: Journal of Molecular Graphics & Modelling (2007), 25(6), 921-927
CODEN: JMGMFI; ISSN: 1093-3263
PUBLISHER: Elsevier Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Three-dimensional quant. structure-activity relationships (3D QSAR) were performed for a series of farsenoid X receptor activators using comparative mol. field anal. (CoMFA). A training set contg. 77 compds. served to establish the models. The best statistical results among all models were obtained with region focusing weighted by a S.D. .times. coeff. values of 0.8 and a grid spacing of 1.0 (r2 = 0.963, SEE = 0.097; q2 = 0.742, SEP = 0.255). The model was used to predict the potency of 20 test set compds. that were not included in the training set, and the predicted values were in good agreement with the exptl. results. The final CoMFA model along with the information obtained from 3D contour maps should be useful for the design of novel FXR ligands having improved potency.
IT ***592524-79-3*** ***592524-80-6*** ***592524-91-9***
592525-09-2 ***592525-32-1*** ***592525-58-1***
592525-81-0 ***592526-01-7*** ***934543-51-8***
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(3D QSAR comparative mol. field anal. on nonsteroidal farnesoid X receptor activators)
RN 592524-79-3 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 72 in file .gra /

RN 592524-80-6 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-ethoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 73 in file .gra /

RN 592524-91-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)(phenylmethyl)amino]phenyl]-,

methyl ester (CA INDEX NAME)

/ Structure 74 in file .gra /

RN 592525-09-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-methoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 75 in file .gra /

RN 592525-32-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2,6-dichlorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 76 in file .gra /

RN 592525-58-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 77 in file .gra /

RN 592525-81-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 78 in file .gra /

RN 592526-01-7 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 79 in file .gra /

RN 934543-51-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[benzoyl[[4-(5-methyl-2-thienyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 80 in file .gra /

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:383580 CAPLUS <<LOGINID::20080729>>
DOCUMENT NUMBER: 144:404429
TITLE: A method using farnesoid X receptor (FXR) agonists with PPAR agonists for reducing drug-induced adverse

side effects in a patient

INVENTOR(S): Fiorucci, Stefano; Pellicciari, Roberto; Pruzanski, Mark

PATENT ASSIGNEE(S): Intercept Pharmaceuticals Inc., USA

SOURCE: PCT Int. Appl., 35 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006044391	A1	20060427	WO 2005-US36536	20051014
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
US 20060252670	A1	20061109	US 2005-250298	20051013
AU 2005295888	A1	20060427	AU 2005-295888	20051014
CA 2584284	A1	20060427	CA 2005-2584284	20051014
EP 1814582	A1	20070808	EP 2005-807696	20051014
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
JP 2008516955	T	20080522	JP 2007-536810	20051014

PRIORITY APPLN. INFO.:

US 2004-619381P	P	20041014
WO 2005-US36536	W	20051014

AB The invention relates to the discovery that farnesoid X receptor (FXR) agonists can be used in combination with peroxisome proliferation activated receptor .gamma. (PPAR.gamma.) agonists to reduce drug-induced adverse side effects in patients suffering from conditions such as insulin resistance, Type II diabetes, metabolic syndrome, non-alc. fatty liver disease (NAFLD), non-alc. steatohepatitis (NASH), and heart disease. Particularly, the invention encompasses methods for treating patients suffering from drug-induced adverse side effects with selective PPAR.gamma., dual PPARa/.gamma. and pan PPAR.alpha./.gamma./.delta. agonists in combination with FXR agonists.

IT ***574013-66-4*** , Fexaramine
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(FXR agonist combination with PPAR agonist for redn. of drug-induced adverse effects)

RN 574013-66-4 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(dimethylamino)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 81 in file .gra /

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1049799 CAPLUS <<LOGINID::20080729>>
DOCUMENT NUMBER: 143:319188
TITLE: Treatment of fibrosis using farnesoid X receptor (FXR) ligands
INVENTOR(S): Fiorucci, Stefano; Pellicciari, Roberto; Pruzanski, Mark
PATENT ASSIGNEE(S): Intercept Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 70 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005089316	A2	20050929	WO 2005-US8575	20050314
WO 2005089316	A3	20060406		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005222994	A1	20050929	AU 2005-222994	20050314
CA 2559476	A1	20050929	CA 2005-2559476	20050314
US 20060069070	A1	20060330	US 2005-81002	20050314
EP 1734970	A2	20061227	EP 2005-729394	20050314
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
JP 2007529427	T	20071025	JP 2007-503111	20050314
PRIORITY APPLN. INFO.:			US 2004-552865P P	20040312
			WO 2005-US8575 W	20050314

AB The invention discloses a method for inhibiting fibrosis that occurs in an organ where the farnesoid X receptor (FXR) is expressed. The method involves administering a high potency, activating ligand of FXR in an effective amt. to a patient who is not suffering from a cholestatic condition. The invention also provides pharmaceutical compns. contg. an effective amt. of an FXR ligand and kits for dispensing the pharmaceutical compns.

IT ***574013-66-4*** , Fexaramine
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(farnesoid X receptor ligands for treatment of fibrosis)

RN 574013-66-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(dimethylamino)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 82 in file .gra /

L8 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:511387 CAPLUS <<LOGINID::20080729>>
DOCUMENT NUMBER: 143:125843
TITLE: Hologram quantitative structure-activity relationships for a series of farnesoid X receptor activators
AUTHOR(S): Honorio, Kathia M.; Garratt, Richard C.; Andricopulo, Adriano D.
CORPORATE SOURCE: Instituto de Fisica de Sao Carlos, Centro de Biotecnologia Molecular Estrutural, Laboratorio de Quimica Medicinal e Computacional, Universidade de Sao Paulo, Sao Carlos-SP, 13560-970, Brazil
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(12), 3119-3125
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The farnesoid X receptor (FXR) is an attractive drug target for the development of novel therapeutic agents for the treatment of dyslipidemia and cholestasis. Hologram quant. structure-activity relationship (HQSAR) studies were conducted on a series of potent FXR activators originated from natural product-like libraries. A training set contg. 82 compds. served to establish the models. The best HQSAR model was generated using atoms, bonds, connections, chirality, and donor and acceptor as fragment distinction and fragment size default (4-7) with six components. The model was used to predict the potency of 20 test set compds. that were not included in the training set, and the predicted values were in good agreement with the exptl. results. The final HQSAR model and the information obtained from HQSAR 2D contribution maps should be useful for the design of novel FXR ligands having improved potency.

IT ***574013-66-4*** ***574013-67-5*** ***592524-78-2***
592524-79-3 ***592524-80-6*** ***592524-85-1***
592524-91-9 ***592524-95-3*** ***592524-96-4***
592525-03-6 ***592525-04-7*** ***592525-05-8***
592525-07-0 ***592525-08-1*** ***592525-09-2***
592525-10-5 ***592525-13-8*** ***592525-21-8***
592525-22-9 ***592525-23-0*** ***592525-25-2***
592525-26-3 ***592525-27-4*** ***592525-32-1***
592525-35-4 ***592525-38-7*** ***592525-47-8***
592525-55-8 ***592525-58-1*** ***592525-61-6***
592525-64-9 ***592525-67-2*** ***592525-78-5***
592525-81-0 ***592525-84-3*** ***592525-90-1***
592525-93-4 ***592525-98-9*** ***592526-01-7***
592526-04-0 ***592526-07-3*** ***592526-12-0***
592526-15-3
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(hologram quant. structure-activity relationships for a series of farnesoid X receptor activators)

RN 574013-66-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(dimethylamino)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 83 in file .gra /

RN 574013-67-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(1,3-benzodioxol-5-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 84 in file .gra /

RN 592524-78-2 CAPLUS
CN 2-Propenoic acid, 3-[4-[[[3-(3-amino-3-oxo-1-propen-1-yl)phenyl](cyclohexylcarbonyl)amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 85 in file .gra /

RN 592524-79-3 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 86 in file .gra /

RN 592524-80-6 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-ethoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 87 in file .gra /

RN 592524-85-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[benzoyl[[4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 88 in file .gra /

RN 592524-91-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)(phenylmethyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 89 in file .gra /

RN 592524-95-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(4-bromophenyl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 90 in file .gra /

RN 592524-96-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(1,1-dimethylethyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 91 in file .gra /

RN 592525-03-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(2-carboxyethenyl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, 1-methyl ester (CA INDEX NAME)

/ Structure 92 in file .gra /

RN 592525-04-7 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 93 in file .gra /

RN 592525-05-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-ethoxy-3-oxo-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 94 in file .gra /

RN 592525-07-0 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, phenylmethyl ester (CA INDEX NAME)

/ Structure 95 in file .gra /

RN 592525-08-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[3-(dimethylamino)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 96 in file .gra /

RN 592525-09-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-methoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 97 in file .gra /

RN 592525-10-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-ethoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 98 in file .gra /

RN 592525-13-8 CAPLUS
CN Benzenepropanoic acid, 4-[[(cyclohexylcarbonyl)[3-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]amino]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 99 in file .gra /

RN 592525-21-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 100 in file .gra /

RN 592525-22-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(3'-acetyl[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 101 in file .gra /

RN 592525-23-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(methylthio)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 102 in file .gra /

RN 592525-25-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(5-methyl-2-thienyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 103 in file .gra /

RN 592525-26-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(5-acetyl-2-thienyl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 104 in file .gra /

RN 592525-27-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methoxyphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 105 in file .gra /

RN 592525-32-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2,6-dichlorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 106 in file .gra /

RN 592525-35-4 CAPLUS

CN 2-Propenoic acid, 3-[3-[[[4-[2-(3-chlorophenyl)ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 107 in file .gra /

RN 592525-38-7 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-[2-[3,5-bis(trifluoromethyl)phenyl]ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 108 in file .gra /

RN 592525-47-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 109 in file .gra /

RN 592525-55-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(3-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 110 in file .gra /

RN 592525-58-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 111 in file .gra /

RN 592525-61-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2-pyridinyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 112 in file .gra /

RN 592525-64-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methyl-5-thiazolyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 113 in file .gra /

RN 592525-67-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3',4'-difluoro[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 114 in file .gra /

RN 592525-78-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-ethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 115 in file .gra /

RN 592525-81-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 116 in file .gra /

RN 592525-84-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(3'-chloro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 117 in file .gra /

RN 592525-90-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 118 in file .gra /

RN 592525-93-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(5'-chloro-2'-methoxy[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 119 in file .gra /

RN 592525-98-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(3'-chloro-4'-fluoro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 120 in file .gra /

RN 592526-01-7 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 121 in file .gra /

RN 592526-04-0 CAPLUS

CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 122 in file .gra /

RN 592526-07-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(2',6'-dimethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 123 in file .gra /

RN 592526-12-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(1,1-dimethylethyl)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 124 in file .gra /

RN 592526-15-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[3-[(1,1-dimethylethyl)amino]-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 125 in file .gra /

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:304966 CAPLUS <<LOGINID::20080729>>
DOCUMENT NUMBER: 143:2829
TITLE: Molecular Dynamics Simulation of the Ligand Binding Domain of Farnesoid X Receptor. Insights into Helix-12 Stability and Coactivator Peptide Stabilization in Response to Agonist Binding
AUTHOR(S): Costantino, Gabriele; Entrena-Guadix, Antonio; Macchiarulo, Antonio; Gioiello, Antimo; Pellicciari, Roberto
CORPORATE SOURCE: Dipartimento di Chimica e Tecnologia del Farmaco, Universita di Perugia, Perugia, 06123, Italy
SOURCE: Journal of Medicinal Chemistry (2005), 48(9), 3251-3259
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The dynamic changes which take place in the ligand binding domain (LBD) of farnesoid X receptor (FXR) in response to agonist binding and in the presence of coactivator peptides were studied with nanosecond time-scale mol. dynamics. Four different systems were analyzed, including the holo-LBD complexed with 6ECDCA, the holo-LBD in the presence of two coactivator peptides, and two artificial apo forms, with and without coactivator peptides. Our results revealed a detailed picture of the differential micro- and macromodifications occurring in the LBD in the

presence or not of the agonist mol. and the coactivator peptides. In the apo simulation a major conformational change took place in the crucial helix 12, while the holo-LBD was globally stabilized by the ligand. When the coactivator peptides were included in the simulation, a clear agonist-induced stabilization was obsd. for the canonical peptide. Interestingly, the second peptide was released from the holo-LBD while it was kept bound in the apo simulation. The present results provide a mol. basis for the understanding the role played by the bile acid agonist in receptor stabilization and enhanced cofactor recruitments.

IT ***574013-66-4*** , Fexaramine
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(mol. dynamics simulation of ligand binding domain of farnesoid X receptor)
RN 574013-66-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(dimethylamino)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 126 in file .gra /

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:453343 CAPLUS <<LOGINID::20080729>>
DOCUMENT NUMBER: 141:19434
TITLE: Crystal structure of the human farnesoid X receptor ligand binding domain complexed with fexaramine and identification and development of novel small molecule ligands for FXR
INVENTOR(S): Downes, Michael R.; Verdicia, Mark A.; Noel, Joseph P.; Evans, Ronald M.; Bowman, Lindsey J.; Bowman, Marianne
PATENT ASSIGNEE(S): The Salk Institute for Biological Studies, USA
SOURCE: PCT Int. Appl., 139 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004046323	A2	20040603	WO 2003-US36548	20031114
WO 2004046323	A3	20041209		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003298654	A1	20040615	AU 2003-298654	20031114
US 20060194949	A1	20060831	US 2005-535042	20050513

PRIORITY APPLN. INFO.: US 2002-426665P P 20021115
US 2002-426668P P 20021115
WO 2003-US36548 W 20031114

AB The present invention provides compns. comprising the ligand binding domain (LBD) of a human farnesoid X receptor (FXR) in cryst. form. In alternative embodiments, the LBD of FXR is complexed with a ligand therefor. There are provided high resoln. structures and structure coordinates of FXR complexed with a novel high affinity agonist, fexaramine. The discovered structure of a FXR LBD provides the first three-dimensional view of the structural basis for FXR ligand binding. The present invention further provides a computer for producing a three-dimensional representation of FXR or a complex thereof, and a computer for detg. at least a portion of the structure coordinates of FXR or a complex thereof. The present invention further provides methods of using this structural information to predict mols. capable of binding to FXR; to identify compds. with agonist, antagonist or partial agonist activity for FXR; and to det. whether a test compd. is capable of binding to the LBD of FXR. The present invention further provides compns. comprising compds. identified by such invention methods. Identification and development of novel small mol. ligands for FXR, and activation of FXR and induction of FXR target genes by these novel compds. is disclosed.

IT ***574013-67-5P*** , Fexarine ***574013-68-6P*** , Fexarene
RL: BSU (Biological study, unclassified); CPN (Combinatorial preparation); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)
(FXR ligand; crystal structure of human farnesoid X receptor ligand binding domain complexed with fexaramine and identification and development of novel small mol. ligands for FXR)

RN 574013-67-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(1,3-benzodioxol-5-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 127 in file .gra /

RN 574013-68-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(2-phenylethenyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 128 in file .gra /

IT ***574013-66-4D*** , Fexaramine, complexes with farnesoid X receptor
RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); BIOL (Biological study); USES (Uses)
(crystal structure of human farnesoid X receptor ligand binding domain complexed with fexaramine and identification and development of novel small mol. ligands for FXR)

RN 574013-66-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(dimethylamino)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 129 in file .gra /

L8 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:453231 CAPLUS <<LOGINID::20080729>>
DOCUMENT NUMBER: 141:23422
TITLE: Preparation of non-steroidal FXR agonists
INVENTOR(S): Nicolaou, Kyriacos C.; Roecker, Anthony J.; Hughes, Robert; Pfefferkorn, Jeffrey A.
PATENT ASSIGNEE(S): The Scripps Research Institute, USA
SOURCE: PCT Int. Appl., 75 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004046162	A2	20040603	WO 2003-US36195	20031114
WO 2004046162	A3	20040812		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003290796	A1	20040615	AU 2003-290796	20031114

PRIORITY APPLN. INFO.:	US 2002-426456P	P	20021114
	US 2003-491185P	P	20030729
	WO 2003-US36195	W	20031114

OTHER SOURCE(S): MARPAT 141:23422
GI

/ Structure 130 in file .gra /

AB Non-steroidal N-aryl-N-arylmethyl amido and ureido compds. such as I [E1 = (C1-C8)alkyl, cyclohexyl, 2-furyl, 3-furyl, 2-thienyl, 3-thienyl, Ph, NH(C1-C8)alkyl; L1, L2 = H; dashed bond = single bond or double bond; X1 = CO, CH2; Y1 = H, NHZ1, NH(Z2)Z3, OZ4; A1 = aryl, heterocyclyl etc.; Z1 = H, Ph, alkyl, benzyl, benzoyl; Z2, Z3 = alkyl; Z2Z3 = cycloalkyl; Z4 = H, oxygen protecting group], were prepd. for their therapeutic use as farnesoid X receptor (FXR) agonists. Thus, biaryl compd. II, prepd. via solid phase synthesis starting from N-(tert-butoxycarbonyl)-3-aminocinnamic acid, Merrifield Resin, 4-bromobenzaldehyde, cyclohexanoyl chloride, and 3,4-difluorobenzeneboronic acid, showed FXR activity (EC50 = 72 nM) and relative efficacy = 1.70 at 1-100 mM CDCA from a cell-based assay. The FXR agonists are useful as therapeutic agents for the treatment of diseases linked to cholesterol, bile acids, and their metab. and homeostasis.
IT ***574013-68-6P***
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)

(prepn. of N-aryl-N-arylmethyl amido and ureido compds. as farnesoid X receptor agonists)
RN 574013-68-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(2-phenylethenyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 131 in file .gra /

IT ***574013-66-4P*** ***574013-67-5P*** ***592525-21-8P***
592525-23-0P ***592525-29-6P*** ***592525-32-1P***
592525-35-4P ***592525-38-7P*** ***592525-41-2P***
592525-44-5P ***592525-47-8P*** ***592525-50-3P***
592525-55-8P ***592525-58-1P*** ***592525-61-6P***
592525-64-9P ***592525-67-2P*** ***592525-72-9P***
592525-78-5P ***592525-81-0P*** ***592525-84-3P***
592525-87-6P ***592525-90-1P*** ***592525-93-4P***
592525-98-9P ***592526-01-7P*** ***592526-04-0P***
592526-07-3P ***592526-12-0P***
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)
(prepn. of N-aryl-N-arylmethyl amido and ureido compds. as farnesoid X receptor agonists)
RN 574013-66-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(dimethylamino)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 132 in file .gra /

RN 574013-67-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(1,3-benzodioxol-5-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 133 in file .gra /

RN 592525-21-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 134 in file .gra /

RN 592525-23-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(methylthio)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 135 in file .gra /

RN 592525-29-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methylphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 136 in file .gra /

RN 592525-32-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2,6-dichlorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 137 in file .gra /

RN 592525-35-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-[2-(3-chlorophenyl)ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 138 in file .gra /

RN 592525-38-7 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-[2-[3,5-bis(trifluoromethyl)phenyl]ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 139 in file .gra /

RN 592525-41-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-[3-(trifluoromethyl)phenyl]ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 140 in file .gra /

RN 592525-44-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2,6-difluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 141 in file .gra /

RN 592525-47-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 142 in file .gra /

RN 592525-50-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2,4,6-trimethylphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 143 in file .gra /

RN 592525-55-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(3-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 144 in file .gra /

RN 592525-58-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 145 in file .gra /

RN 592525-61-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2-pyridinyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 146 in file .gra /

RN 592525-64-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methyl-5-thiazolyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 147 in file .gra /

RN 592525-67-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3',4'-difluoro[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 148 in file .gra /

RN 592525-72-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(2'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 149 in file .gra /

RN 592525-78-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-ethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 150 in file .gra /

RN 592525-81-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-methoxy[1,1'-biphenyl]-4-

yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 151 in file .gra /

RN 592525-84-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(3'-chloro[1,1'-biphenyl]-4-
yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX
NAME)

/ Structure 152 in file .gra /

RN 592525-87-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-methyl[1,1'-biphenyl]-4-
yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 153 in file .gra /

RN 592525-90-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-methyl[1,1'-biphenyl]-4-
yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 154 in file .gra /

RN 592525-93-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(5'-chloro-2'-methoxy[1,1'-biphenyl]-4-
yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX
NAME)

/ Structure 155 in file .gra /

RN 592525-98-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(3'-chloro-4'-fluoro[1,1'-biphenyl]-4-
yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX
NAME)

/ Structure 156 in file .gra /

RN 592526-01-7 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(trifluoromethoxy)[1,1'-
biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 157 in file .gra /

RN 592526-04-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[3'-(trifluoromethoxy)[1,1'-
biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 158 in file .gra /

RN 592526-07-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(2',6'-dimethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 159 in file .gra /

RN 592526-12-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(1,1-dimethylethyl)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 160 in file .gra /

IT ***592524-75-9P***
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of N-aryl-N-arylmethyl amido and ureido compds. as farnesoid X receptor agonists)
RN 592524-75-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 161 in file .gra /

IT ***592524-76-0P*** ***592524-77-1P*** ***592524-78-2P***
592524-79-3P ***592524-80-6P*** ***592524-81-7P***
592524-85-1P ***592524-91-9P*** ***592524-96-4P***
592525-04-7P ***592525-05-8P*** ***592525-06-9P***
592525-07-0P ***592525-08-1P*** ***592525-09-2P***
592525-10-5P ***592525-11-6P*** ***592525-12-7P***
592525-13-8P ***592525-22-9P*** ***592525-24-1P***
592525-25-2P ***592525-27-4P*** ***592525-28-5P***
592526-15-3P ***698360-00-8P*** ***698363-47-2P***
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-aryl-N-arylmethyl amido and ureido compds. as farnesoid X receptor agonists)
RN 592524-76-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, ethyl ester (CA INDEX NAME)

/ Structure 162 in file .gra /

RN 592524-77-1 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 163 in file .gra /

RN 592524-78-2 CAPLUS
CN 2-Propenoic acid, 3-[4-[[[3-(3-amino-3-oxo-1-propen-1-yl)phenyl](cyclohexylcarbonyl)amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 164 in file .gra /

RN 592524-79-3 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 165 in file .gra /

RN 592524-80-6 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-ethoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 166 in file .gra /

RN 592524-81-7 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-phenoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 167 in file .gra /

RN 592524-85-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[benzoyl[[4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 168 in file .gra /

RN 592524-91-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)(phenylmethyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 169 in file .gra /

RN 592524-96-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(1,1-dimethylethyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 170 in file .gra /

RN 592525-04-7 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 171 in file .gra /

RN 592525-05-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-ethoxy-3-oxo-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 172 in file .gra /

RN 592525-06-9 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1-methylethyl ester (CA INDEX NAME)

/ Structure 173 in file .gra /

RN 592525-07-0 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, phenylmethyl ester (CA INDEX NAME)

/ Structure 174 in file .gra /

RN 592525-08-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[3-(dimethylamino)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 175 in file .gra /

RN 592525-09-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-methoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 176 in file .gra /

RN 592525-10-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-ethoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 177 in file .gra /

RN 592525-11-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-phenoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 178 in file .gra /

RN 592525-12-7 CAPLUS
CN Benzenepropanoic acid, 4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 179 in file .gra /

RN 592525-13-8 CAPLUS
CN Benzenepropanoic acid, 4-[[(cyclohexylcarbonyl)[3-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]amino]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 180 in file .gra /

RN 592525-22-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(3'-acetyl[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 181 in file .gra /

RN 592525-24-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[([1,1'-biphenyl]-4-ylmethyl)(cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 182 in file .gra /

RN 592525-25-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(5-methyl-2-thienyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 183 in file .gra /

RN 592525-27-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methoxyphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 184 in file .gra /

RN 592525-28-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-[4-(1,1-dimethylethyl)phenyl]ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 185 in file .gra /

RN 592526-15-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[3-[(1,1-dimethylethyl)amino]-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 186 in file .gra /

RN 698360-00-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(5-acetyl-2-thienyl)phenyl]methyl][(2-

methylcyclohexyl)carbonyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 187 in file .gra /

RN 698363-47-2 CAPLUS
CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]- (CA INDEX NAME)

/ Structure 188 in file .gra /

IT ***592524-95-3P*** ***592525-03-6P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of N-aryl-N-arylmethyl amido and ureido compds. as farnesoid X receptor agonists)
RN 592524-95-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(4-bromophenyl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 189 in file .gra /

RN 592525-03-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(2-carboxyethenyl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, 1-methyl ester (CA INDEX NAME)

/ Structure 190 in file .gra /

L8 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:453152 CAPLUS <<LOGINID::20080729>>
DOCUMENT NUMBER: 141:17647
TITLE: N-acyl-N-arylmethylaniline acrylates as nonsteroidal farnesoid X receptor modulators
INVENTOR(S): Downes, Michael R.; Evans, Ronald M.
PATENT ASSIGNEE(S): The Salk Institute for Biological Studies, USA
SOURCE: PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004046068	A2	20040603	WO 2003-US36137	20031114
WO 2004046068	A3	20041229		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,

BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 20050143449	A1	20050630	US 2003-658115		20030908
AU 2003294264	A1	20040615	AU 2003-294264		20031114
US 20060128764	A1	20060615	US 2005-535043		20051209
PRIORITY APPLN. INFO.:			US 2002-426664P	P	20021115
			US 2003-658115	A2	20030908
			WO 2003-US36137	W	20031114

OTHER SOURCE(S): MARPAT 141:17647
GI

/ Structure 191 in file .gra /

AB A method for modulating process(es) mediated by farnesyl X receptor polypeptides comprises conducting said process(es) in the presence of title compds. [I; A = (substituted) alkyl, cycloalkyl, aryl, heteroaryl; X = CO, CH2; R = Me, Et; R1 = H, OH, alkoxy, PhCO2, mesityloxy, OCH2CO2Et; R2 = H; R3 = alkenyl, (substituted) aryl, heteroaryl, aralkenyl, heteroaralkenyl; R2R3 = atoms to form a (substituted) (unsatd.) pyran ring; R4 = H, OH; R5 = H, OH, alkoxy, aryloxy]. In a cell-based transcription assay, title compd. (II) activated FXR with EC50 = 36 nM.

IT ***592524-95-3P***
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of N-acyl-N-arylmethylaniline acrylates as nonsteroidal farnesoid X receptor modulators)

RN 592524-95-3 CAPLUS

CN 2-Propenoic acid, 3-[3-[[(4-bromophenyl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 192 in file .gra /

IT

574013-66-4P	***574013-67-5P***	***574013-68-6P***
592524-75-9P	***592524-76-0P***	***592524-77-1P***
592524-78-2P	***592524-79-3P***	***592524-80-6P***
592524-81-7P	***592524-85-1P***	***592524-91-9P***
592524-96-4P	***592525-03-6P***	***592525-04-7P***
592525-05-8P	***592525-06-9P***	***592525-07-0P***
592525-08-1P	***592525-09-2P***	***592525-10-5P***
592525-11-6P	***592525-12-7P***	***592525-13-8P***
592525-21-8P	***592525-22-9P***	***592525-23-0P***
592525-24-1P	***592525-25-2P***	***592525-26-3P***
592525-27-4P	***592525-28-5P***	***592525-29-6P***
592525-32-1P	***592525-35-4P***	***592525-38-7P***
592525-41-2P	***592525-44-5P***	***592525-47-8P***
592525-50-3P	***592525-55-8P***	***592525-58-1P***
592525-61-6P	***592525-64-9P***	***592525-67-2P***
592525-72-9P	***592525-78-5P***	***592525-81-0P***
592525-84-3P	***592525-87-6P***	***592525-90-1P***
592525-93-4P	***592525-98-9P***	***592526-01-7P***

592526-04-0P ***592526-07-3P*** ***592526-12-0P***
592526-16-4P ***699006-40-1P*** ***699006-41-2P***
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-acyl-N-arylmethylaniline acrylates as nonsteroidal farnesoid X receptor modulators)

RN 574013-66-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(dimethylamino)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 193 in file .gra /

RN 574013-67-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(1,3-benzodioxol-5-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 194 in file .gra /

RN 574013-68-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(2-phenylethenyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 195 in file .gra /

RN 592524-75-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 196 in file .gra /

RN 592524-76-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, ethyl ester (CA INDEX NAME)

/ Structure 197 in file .gra /

RN 592524-77-1 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 198 in file .gra /

RN 592524-78-2 CAPLUS
CN 2-Propenoic acid, 3-[4-[[[3-(3-amino-3-oxo-1-propen-1-yl)phenyl](cyclohexylcarbonyl)amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 199 in file .gra /

RN 592524-79-3 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 200 in file .gra /

RN 592524-80-6 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-ethoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 201 in file .gra /

RN 592524-81-7 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-phenoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 202 in file .gra /

RN 592524-85-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[benzoyl[[4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 203 in file .gra /

RN 592524-91-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)(phenylmethyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 204 in file .gra /

RN 592524-96-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(1,1-dimethylethyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 205 in file .gra /

RN 592525-03-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(2-carboxyethenyl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, 1-methyl ester (CA INDEX NAME)

/ Structure 206 in file .gra /

RN 592525-04-7 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 207 in file .gra /

RN 592525-05-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-ethoxy-3-oxo-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 208 in file .gra /

RN 592525-06-9 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1-methylethyl ester (CA INDEX NAME)

/ Structure 209 in file .gra /

RN 592525-07-0 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, phenylmethyl ester (CA INDEX NAME)

/ Structure 210 in file .gra /

RN 592525-08-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[3-(dimethylamino)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 211 in file .gra /

RN 592525-09-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-methoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 212 in file .gra /

RN 592525-10-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-ethoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 213 in file .gra /

RN 592525-11-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-phenoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 214 in file .gra /

RN 592525-12-7 CAPLUS
CN Benzenepropanoic acid, 4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 215 in file .gra /

RN 592525-13-8 CAPLUS
CN Benzenepropanoic acid, 4-[[(cyclohexylcarbonyl)[3-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]amino]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 216 in file .gra /

RN 592525-21-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 217 in file .gra /

RN 592525-22-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(3'-acetyl[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 218 in file .gra /

RN 592525-23-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(methylthio)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 219 in file .gra /

RN 592525-24-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[([1,1'-biphenyl]-4-ylmethyl)(cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 220 in file .gra /

RN 592525-25-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(5-methyl-2-thienyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 221 in file .gra /

RN 592525-26-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(5-acetyl-2-thienyl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 222 in file .gra /

RN 592525-27-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methoxyphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA

INDEX NAME)

/ Structure 223 in file .gra /

RN 592525-28-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-[4-(1,1-dimethylethyl)phenyl]ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 224 in file .gra /

RN 592525-29-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methylphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 225 in file .gra /

RN 592525-32-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2,6-dichlorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 226 in file .gra /

RN 592525-35-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-[2-(3-chlorophenyl)ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 227 in file .gra /

RN 592525-38-7 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-[2-[3,5-bis(trifluoromethyl)phenyl]ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 228 in file .gra /

RN 592525-41-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-[3-(trifluoromethyl)phenyl]ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 229 in file .gra /

RN 592525-44-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2,6-difluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 230 in file .gra /

RN 592525-47-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 231 in file .gra /

RN 592525-50-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2,4,6-trimethylphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 232 in file .gra /

RN 592525-55-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(3-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 233 in file .gra /

RN 592525-58-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 234 in file .gra /

RN 592525-61-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2-pyridinyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 235 in file .gra /

RN 592525-64-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methyl-5-thiazolyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 236 in file .gra /

RN 592525-67-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3',4'-difluoro[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 237 in file .gra /

RN 592525-72-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(2'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 238 in file .gra /

RN 592525-78-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-ethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 239 in file .gra /

RN 592525-81-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 240 in file .gra /

RN 592525-84-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(3'-chloro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 241 in file .gra /

RN 592525-87-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 242 in file .gra /

RN 592525-90-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 243 in file .gra /

RN 592525-93-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(5'-chloro-2'-methoxy[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 244 in file .gra /

RN 592525-98-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(3'-chloro-4'-fluoro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 245 in file .gra /

RN 592526-01-7 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 246 in file .gra /

RN 592526-04-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 247 in file .gra /

RN 592526-07-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(2',6'-dimethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 248 in file .gra /

RN 592526-12-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(1,1-dimethylethyl)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 249 in file .gra /

RN 592526-16-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3',5'-dichloro[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 250 in file .gra /

RN 699006-40-1 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 2-methylpropyl ester (CA INDEX NAME)

/ Structure 251 in file .gra /

RN 699006-41-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[3-[(2-methylpropyl)amino]-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 252 in file .gra /

L8 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:452954 CAPLUS <<LOGINID::20080729>>
DOCUMENT NUMBER: 141:17646

TITLE: N-acyl-N-benzylaniline acrylates as nonsteroidal farnesoid X receptor (FXR) modulators

INVENTOR(S): Downes, Michael R.; Evans, Ronald Mark; Hughes, Robert; Nicolaou, Kyriacos C.; Roecker, Anthony J.

PATENT ASSIGNEE(S): The Salk Institute for Biological Studies, USA; The Scripps Research Institute

SOURCE: PCT Int. Appl., 62 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004045511	A2	20040603	WO 2003-US36123	20031114
WO 2004045511	A3	20040708		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20050143449	A1	20050630	US 2003-658115	20030908
AU 2003290778	A1	20040615	AU 2003-290778	20031114
US 20060223879	A1	20061005	US 2005-535041	20051228

PRIORITY APPLN. INFO.:

US 2002-426664P	P	20021115
US 2003-658115	A2	20030908
WO 2003-US36123	W	20031114

OTHER SOURCE(S): MARPAT 141:17646

GI

/ Structure 253 in file .gra /

AB Title compds. [I; A = (substituted) alkyl, cycloalkyl, aryl, heteroaryl; X = CO, CH2; R = Me, Et; R1 = H, OH, alkoxy, PhCO2, mesityloxy, OCH2CO2Et; R2 = H; R3 = alkenyl, (substituted) aryl, heteroaryl, aralkenyl, heteroaralkenyl; R2R3 = atoms to form a substituted (unsatd.) pyran ring; R4 = H, OH; R5 = H, OH, alkoxy, aryloxy], are claimed. Thus, benzopyran deriv. (II) activated FXR receptors with EC50 = 358 nM.

IT ***592524-95-3P***
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of acylbenzylaniline acrylates as nonsteroidal farnesoid X receptor (FXR) modulators)

RN 592524-95-3 CAPLUS

CN 2-Propenoic acid, 3-[3-[[(4-bromophenyl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 254 in file .gra /

IT ***574013-66-4P*** ***574013-67-5P*** ***574013-68-6P***
592524-75-9P ***592524-76-0P*** ***592524-77-1P***
592524-78-2P ***592524-79-3P*** ***592524-80-6P***
592524-81-7P ***592524-85-1P*** ***592524-91-9P***
592524-96-4P ***592525-03-6P*** ***592525-04-7P***
592525-05-8P ***592525-06-9P*** ***592525-07-0P***
592525-08-1P ***592525-09-2P*** ***592525-10-5P***
592525-11-6P ***592525-12-7P*** ***592525-21-8P***
592525-22-9P ***592525-23-0P*** ***592525-24-1P***
592525-25-2P ***592525-26-3P*** ***592525-27-4P***
592525-28-5P ***592525-29-6P*** ***592525-32-1P***
592525-35-4P ***592525-38-7P*** ***592525-41-2P***
592525-44-5P ***592525-47-8P*** ***592525-50-3P***
592525-55-8P ***592525-58-1P*** ***592525-61-6P***
592525-64-9P ***592525-67-2P*** ***592525-72-9P***
592525-78-5P ***592525-81-0P*** ***592525-84-3P***
592525-87-6P ***592525-90-1P*** ***592525-93-4P***
592525-98-9P ***592526-01-7P*** ***592526-04-0P***
592526-07-3P ***592526-12-0P*** ***592526-15-3P***
592526-16-4P ***699021-26-6P***
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of acylbenzylaniline acrylates as nonsteroidal farnesoid X receptor (FXR) modulators)
RN 574013-66-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(dimethylamino)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 255 in file .gra /

RN 574013-67-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(1,3-benzodioxol-5-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 256 in file .gra /

RN 574013-68-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(2-phenylethenyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 257 in file .gra /

RN 592524-75-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 258 in file .gra /

RN 592524-76-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, ethyl ester (CA INDEX NAME)

/ Structure 259 in file .gra /

RN 592524-77-1 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 260 in file .gra /

RN 592524-78-2 CAPLUS
CN 2-Propenoic acid, 3-[4-[[[3-(3-amino-3-oxo-1-propen-1-yl)phenyl](cyclohexylcarbonyl)amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 261 in file .gra /

RN 592524-79-3 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 262 in file .gra /

RN 592524-80-6 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-ethoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 263 in file .gra /

RN 592524-81-7 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-phenoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 264 in file .gra /

RN 592524-85-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[benzoyl[[4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 265 in file .gra /

RN 592524-91-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)(phenylmethyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 266 in file .gra /

RN   592524-96-4 CAPLUS
CN   2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(1,1-
     dimethylethyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 267 in file .gra /

RN   592525-03-6 CAPLUS
CN   2-Propenoic acid, 3-[3-[[[4-(2-carboxyethenyl)phenyl]methyl](cyclohexylcar
     bonyl)amino]phenyl]-, 1-methyl ester (CA INDEX NAME)

/ Structure 268 in file .gra /

RN   592525-04-7 CAPLUS
CN   2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-
     1-yl)phenyl]amino]methyl]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 269 in file .gra /

RN   592525-05-8 CAPLUS
CN   2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-ethoxy-3-oxo-1-propen-1-
     yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 270 in file .gra /

RN   592525-06-9 CAPLUS
CN   2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-
     1-yl)phenyl]amino]methyl]phenyl]-, 1-methylethyl ester (CA INDEX NAME)

/ Structure 271 in file .gra /

RN   592525-07-0 CAPLUS
CN   2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-
     1-yl)phenyl]amino]methyl]phenyl]-, phenylmethyl ester (CA INDEX NAME)

/ Structure 272 in file .gra /

RN   592525-08-1 CAPLUS
CN   2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[3-(dimethylamino)-3-oxo-1-
     propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 273 in file .gra /

RN   592525-09-2 CAPLUS
CN   2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-methoxy-1-propen-1-
     yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 274 in file .gra /

RN 592525-10-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-ethoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 275 in file .gra /

RN 592525-11-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-phenoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 276 in file .gra /

RN 592525-12-7 CAPLUS
CN Benzenepropanoic acid, 4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 277 in file .gra /

RN 592525-21-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 278 in file .gra /

RN 592525-22-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(3'-acetyl[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 279 in file .gra /

RN 592525-23-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(methylthio)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 280 in file .gra /

RN 592525-24-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[([1,1'-biphenyl]-4-ylmethyl)(cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 281 in file .gra /

RN 592525-25-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(5-methyl-2-thienyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 282 in file .gra /

RN 592525-26-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(5-acetyl-2-thienyl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 283 in file .gra /

RN 592525-27-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methoxyphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 284 in file .gra /

RN 592525-28-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-[4-(1,1-dimethylethyl)phenyl]ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 285 in file .gra /

RN 592525-29-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methylphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 286 in file .gra /

RN 592525-32-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2,6-dichlorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 287 in file .gra /

RN 592525-35-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-[2-(3-chlorophenyl)ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 288 in file .gra /

RN 592525-38-7 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-[2-[3,5-bis(trifluoromethyl)phenyl]ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 289 in file .gra /

RN 592525-41-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-[3-(trifluoromethyl)phenyl]ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 290 in file .gra /

RN 592525-44-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2,6-difluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 291 in file .gra /

RN 592525-47-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 292 in file .gra /

RN 592525-50-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2,4,6-trimethylphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 293 in file .gra /

RN 592525-55-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(3-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 294 in file .gra /

RN 592525-58-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 295 in file .gra /

RN 592525-61-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2-pyridinyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 296 in file .gra /

RN 592525-64-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methyl-5-thiazolyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 297 in file .gra /

RN 592525-67-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3',4'-difluoro[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 298 in file .gra /

RN 592525-72-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(2'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 299 in file .gra /

RN 592525-78-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-ethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 300 in file .gra /

RN 592525-81-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 301 in file .gra /

RN 592525-84-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(3'-chloro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 302 in file .gra /

RN 592525-87-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 303 in file .gra /

RN 592525-90-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 304 in file .gra /

RN 592525-93-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(5'-chloro-2'-methoxy[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 305 in file .gra /

RN 592525-98-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(3'-chloro-4'-fluoro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 306 in file .gra /

RN 592526-01-7 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 307 in file .gra /

RN 592526-04-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 308 in file .gra /

RN 592526-07-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(2',6'-dimethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 309 in file .gra /

RN 592526-12-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(1,1-dimethylethyl)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 310 in file .gra /

RN 592526-15-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[3-[(1,1-dimethylethyl)amino]-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 311 in file .gra /

RN 592526-16-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3',5'-dichloro[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 312 in file .gra /

RN 699021-26-6 CAPLUS
CN Benzenepropanoic acid, 4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]-, methyl ester (CA INDEX NAME)

/ Structure 313 in file .gra /

L8 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:375244 CAPLUS <<LOGINID::20080729>>
DOCUMENT NUMBER: 139:159454
TITLE: A chemical, genetic, and structural analysis of the nuclear bile acid receptor FXR
AUTHOR(S): Downes, Michael; Verdecia, Mark A.; Roecker, A. J.; Hughes, Robert; Hogenesch, John B.; Kast-Woelbern, Heidi R.; Bowman, Marianne E.; Ferrer, Jean-Luc; Anisfeld, Andrew M.; Edwards, Peter A.; Rosenfeld, John M.; Alvarez, Jacqueline G. A.; Noel, Joseph P.; Nicolaou, K. C.; Evans, Ronald M.
CORPORATE SOURCE: Gene Expression Laboratory, Howard Hughes Medical Institute, La Jolla, CA, 92037, USA
SOURCE: Molecular Cell (2003), 11(4), 1079-1092
CODEN: MOCEFL; ISSN: 1097-2765
PUBLISHER: Cell Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The farnesoid X receptor (FXR) functions as a bile acid (BA) sensor coordinating cholesterol metab., lipid homeostasis, and absorption of dietary fats and vitamins. However, BAs are poor reagents for characterizing FXR functions due to multiple receptor independent properties. Accordingly, using combinatorial chem. we evolved a small mol. agonist termed fexaramine with 100-fold increased affinity relative to natural compds. Gene-profiling expts. conducted in hepatocytes with FXR-specific fexaramine vs. the primary BA chenodeoxycholic acid (CDCA) produced remarkably distinct genomic targets. Highly diffracting cocrystals (1.78 .ANG.) of fexaramine bound to the ligand binding domain of FXR revealed the agonist sequestered in a 726 .ANG.3 hydrophobic cavity and suggest a mechanistic basis for the initial step in the BA signaling pathway. The discovery of fexaramine will allow us to unravel the FXR genetic network from the BA network and selectively manipulate components of the cholesterol pathway that may be useful in treating cholesterol-related human diseases.
IT ***574013-66-4P*** , Fexaramine ***574013-67-5P*** , Fexarine ***574013-68-6P*** , Fexarene
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(chem., genetic, and structural anal. of nuclear bile acid receptor FXR)
RN 574013-66-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(dimethylamino)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 314 in file .gra /

RN 574013-67-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(1,3-benzodioxol-5-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 315 in file .gra /

RN 574013-68-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(2-phenylethenyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 316 in file .gra /

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:354702 CAPLUS <<LOGINID::20080729>>
DOCUMENT NUMBER: 139:224366
TITLE: Discovery and optimization of non-steroidal FXR agonists from natural product-like libraries
AUTHOR(S): Nicolaou, K. C.; Evans, Ronald M.; Roecker, A. J.; Hughes, Robert; Downes, Michael; Pfefferkorn, Jeffery A.
CORPORATE SOURCE: Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Organic & Biomolecular Chemistry (2003), 1(6), 908-920
CODEN: OBCRAK; ISSN: 1477-0520
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The efficient regulation of cholesterol biosynthesis, metab., acquisition, and transport is an essential component of lipid homeostasis. The farnesoid X receptor (FXR) is a transcriptional sensor for bile acids, the primary product of cholesterol metab. Accordingly, the development of potent, selective, small mol. agonists, partial agonists, and antagonists of FXR would be an important step in further deconvoluting FXR physiol. Herein, we describe the development of four novel classes of potent FXR activators originating from natural product-like libraries. Initial screening of a 10000-membered, diversity-orientated library of benzopyran contg. small mols. for FXR activation utilizing a cell-based reporter assay led to the identification of several lead compds. possessing low micromolar activity (EC50's = 5-10 .mu.M). These compds. were systematically optimized employing parallel soln.-phase synthesis and solid-phase synthesis to provide four classes of compds. that potently activate FXR. Two series of compds., bearing stilbene or biaryl moieties, contain members that are the most potent FXR agonists reported to date in cell-based assays. These compds. may find future utility as chem. tools in studies aimed at further defining the physiol. role of FXR and discovering potential therapeutic agents for the treatment of diseases linked to cholesterol and bile acid metab. and homeostasis.
IT ***574013-66-4*** ***574013-67-5*** ***574013-68-6***

592524-75-9 ***592524-76-0*** ***592524-77-1***
592524-78-2 ***592524-79-3*** ***592524-80-6***
592524-81-7 ***592524-85-1*** ***592524-91-9***
592524-95-3 ***592524-96-4*** ***592525-03-6***
592525-04-7 ***592525-05-8*** ***592525-06-9***
592525-07-0 ***592525-08-1*** ***592525-09-2***
592525-10-5 ***592525-11-6*** ***592525-12-7***
592525-13-8 ***592525-21-8*** ***592525-22-9***
592525-23-0 ***592525-24-1*** ***592525-25-2***
592525-26-3 ***592525-27-4*** ***592525-28-5***
592525-29-6 ***592525-32-1*** ***592525-35-4***
592525-38-7 ***592525-41-2*** ***592525-44-5***
592525-47-8 ***592525-50-3*** ***592525-55-8***
592525-58-1 ***592525-61-6*** ***592525-64-9***
592525-67-2 ***592525-72-9*** ***592525-78-5***
592525-81-0 ***592525-84-3*** ***592525-87-6***
592525-90-1 ***592525-93-4*** ***592525-98-9***
592526-01-7 ***592526-04-0*** ***592526-07-3***
592526-12-0 ***592526-15-3*** ***592526-16-4***

RL: PAC (Pharmacological activity); BIOL (Biological study)
(discovery and optimization of non-steroidal FXR agonists from natural product-like libraries)

RN 574013-66-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(dimethylamino)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 317 in file .gra /

RN 574013-67-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(1,3-benzodioxol-5-yl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 318 in file .gra /

RN 574013-68-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(2-phenylethenyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 319 in file .gra /

RN 592524-75-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 320 in file .gra /

RN 592524-76-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, ethyl ester (CA INDEX NAME)

/ Structure 321 in file .gra /

RN 592524-77-1 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 322 in file .gra /

RN 592524-78-2 CAPLUS
CN 2-Propenoic acid, 3-[4-[[[3-(3-amino-3-oxo-1-propen-1-yl)phenyl](cyclohexylcarbonyl)amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 323 in file .gra /

RN 592524-79-3 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 324 in file .gra /

RN 592524-80-6 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-ethoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 325 in file .gra /

RN 592524-81-7 CAPLUS
CN 2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-phenoxy-1-propen-1-yl)phenyl]amino]methyl]phenyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 326 in file .gra /

RN 592524-85-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[benzoyl[[4-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 327 in file .gra /

RN 592524-91-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)(phenylmethyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 328 in file .gra /

RN 592524-95-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(4-bromophenyl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 329 in file .gra /

RN   592524-96-4 CAPLUS
CN   2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(1,1-
     dimethylethyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 330 in file .gra /

RN   592525-03-6 CAPLUS
CN   2-Propenoic acid, 3-[3-[[[4-(2-carboxyethenyl)phenyl]methyl](cyclohexylcar
     bonyl)amino]phenyl]-, 1-methyl ester (CA INDEX NAME)

/ Structure 331 in file .gra /

RN   592525-04-7 CAPLUS
CN   2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-
     1-yl)phenyl]amino]methyl]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 332 in file .gra /

RN   592525-05-8 CAPLUS
CN   2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-ethoxy-3-oxo-1-propen-1-
     yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 333 in file .gra /

RN   592525-06-9 CAPLUS
CN   2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-
     1-yl)phenyl]amino]methyl]phenyl]-, 1-methylethyl ester (CA INDEX NAME)

/ Structure 334 in file .gra /

RN   592525-07-0 CAPLUS
CN   2-Propenoic acid, 3-[4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-
     1-yl)phenyl]amino]methyl]phenyl]-, phenylmethyl ester (CA INDEX NAME)

/ Structure 335 in file .gra /

RN   592525-08-1 CAPLUS
CN   2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[3-(dimethylamino)-3-oxo-1-
     propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 336 in file .gra /

RN   592525-09-2 CAPLUS
CN   2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-methoxy-1-propen-1-
     yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 337 in file .gra /

RN 592525-10-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-ethoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 338 in file .gra /

RN 592525-11-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(3-phenoxy-1-propen-1-yl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 339 in file .gra /

RN 592525-12-7 CAPLUS
CN Benzenepropanoic acid, 4-[[(cyclohexylcarbonyl)[3-(3-methoxy-3-oxo-1-propen-1-yl)phenyl]amino]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 340 in file .gra /

RN 592525-13-8 CAPLUS
CN Benzenepropanoic acid, 4-[[(cyclohexylcarbonyl)[3-[3-(1,1-dimethylethoxy)-3-oxo-1-propen-1-yl]phenyl]amino]methyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

/ Structure 341 in file .gra /

RN 592525-21-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 342 in file .gra /

RN 592525-22-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(3'-acetyl[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 343 in file .gra /

RN 592525-23-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(methylthio)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 344 in file .gra /

RN 592525-24-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[([1,1'-biphenyl]-4-ylmethyl)(cyclohexylcarbonyl)am

ino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 345 in file .gra /

RN 592525-25-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-(5-methyl-2-thienyl)phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 346 in file .gra /

RN 592525-26-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-(5-acetyl-2-thienyl)phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 347 in file .gra /

RN 592525-27-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methoxyphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 348 in file .gra /

RN 592525-28-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-[4-(1,1-dimethylethyl)phenyl]ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 349 in file .gra /

RN 592525-29-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methylphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 350 in file .gra /

RN 592525-32-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2,6-dichlorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 351 in file .gra /

RN 592525-35-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-[2-(3-chlorophenyl)ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 352 in file .gra /

RN 592525-38-7 CAPLUS
CN 2-Propenoic acid, 3-[3-[[[4-[2-[3,5-bis(trifluoromethyl)phenyl]ethenyl]phenyl]methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 353 in file .gra /

RN 592525-41-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-[3-(trifluoromethyl)phenyl]ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 354 in file .gra /

RN 592525-44-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2,6-difluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 355 in file .gra /

RN 592525-47-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 356 in file .gra /

RN 592525-50-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2,4,6-trimethylphenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 357 in file .gra /

RN 592525-55-8 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(3-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 358 in file .gra /

RN 592525-58-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-fluorophenyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 359 in file .gra /

RN 592525-61-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(2-pyridinyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 360 in file .gra /

RN 592525-64-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[2-(4-methyl-5-thiazolyl)ethenyl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 361 in file .gra /

RN 592525-67-2 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3',4'-difluoro[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 362 in file .gra /

RN 592525-72-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(2'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 363 in file .gra /

RN 592525-78-5 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-ethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 364 in file .gra /

RN 592525-81-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-methoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 365 in file .gra /

RN 592525-84-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(3'-chloro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 366 in file .gra /

RN 592525-87-6 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(4'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 367 in file .gra /

RN 592525-90-1 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3'-methyl[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 368 in file .gra /

RN 592525-93-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(5'-chloro-2'-methoxy[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 369 in file .gra /

RN 592525-98-9 CAPLUS
CN 2-Propenoic acid, 3-[3-[[(3'-chloro-4'-fluoro[1,1'-biphenyl]-4-yl)methyl](cyclohexylcarbonyl)amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 370 in file .gra /

RN 592526-01-7 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 371 in file .gra /

RN 592526-04-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 372 in file .gra /

RN 592526-07-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(2',6'-dimethoxy[1,1'-biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 373 in file .gra /

RN 592526-12-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4'-(1,1-dimethylethyl)[1,1'-biphenyl]-4-yl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 374 in file .gra /

RN 592526-15-3 CAPLUS
CN 2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[[4-[3-[(1,1-dimethylethyl)amino]-3-oxo-1-propen-1-yl]phenyl]methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 375 in file .gra /

RN   592526-16-4 CAPLUS
CN   2-Propenoic acid, 3-[3-[(cyclohexylcarbonyl)[(3',5'-dichloro[1,1'-
     biphenyl]-4-yl)methyl]amino]phenyl]-, methyl ester (CA INDEX NAME)

/ Structure 376 in file .gra /

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                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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